## LSTM-based Neural Networks for Slurry Deformation Prediction: A Bayesian Optimization Approach

ABSTRACT

This dissertation presents a comprehensive investigation into the application of Long Short-Term Memory (LSTM) networks for predicting slurry deformation. The study utilizes a hybrid approach, combining traditional machine learning techniques with Bayesian optimization, to develop a robust and highly accurate predictive model. The dissertation explores the intricacies of LSTM architecture, data augmentation techniques, and hyperparameter optimization methodologies. It evaluates the model's performance using various metrics such as mean squared error (MSE), mean absolute error (MAE), and R-squared (R²) on a real-world dataset. The results demonstrate the effectiveness of the proposed approach, achieving superior prediction accuracy compared to baseline models. Furthermore, the dissertation contributes to the field by offering insights into the influence of various hyperparameters on model performance, enabling researchers and practitioners to optimize their LSTM models for specific applications.

1. INTRODUCTION

1.1. Motivation:

The motivation for this research stems from several factors:

* Need for accurate and reliable slurry deformation prediction: Traditional methods often fail to capture the complex interactions within slurries, leading to inaccurate predictions and potential operational issues.
* Efficiency and cost-effectiveness: Data-driven models can significantly reduce the need for expensive and time-consuming experiments, offering a cost-effective solution for optimizing slurry handling.
* Improved process control and safety: Accurate deformation predictions enable better control over slurry behavior, reducing risks associated with pipe blockages, equipment wear, and environmental hazards.

1.2. Research Objectives:

This dissertation aims to achieve the following objectives:

1. Develop a robust and accurate LSTM-based model for slurry deformation prediction.
2. Investigate the impact of data augmentation techniques on model performance.
3. Optimize hyperparameters of the LSTM network using Bayesian optimization.
4. Evaluate the model's performance using various metrics and compare it with baseline models.
5. Analyze the influence of key hyperparameters on model accuracy and generalization ability.
6. Offer insights into the advantages and limitations of using LSTM networks for slurry deformation prediction.

2. BACKGROUND AND LITERATURE REVIEW:

This section provides an overview of the relevant background and literature related to slurry deformation prediction, LSTM networks, and Bayesian optimization.

2.1. Slurry Deformation:

Slurry deformation is a complex phenomenon influenced by various factors, including:

* Solid particle size and distribution: The size, shape, and concentration of solid particles significantly affect the rheological properties of slurries.
* Fluid properties: The viscosity and density of the liquid phase impact the flow behavior and deformation characteristics.
* Shear rate and stress: The rate of deformation and applied stress influence the slurry's response and potential for yielding.
* Temperature and pressure: External conditions can alter the fluid properties and particle interactions, leading to changes in deformation behavior.

2.2. LSTM Networks:

LSTM networks are a type of recurrent neural network (RNN) specifically designed to handle sequential data with long-term dependencies. They employ internal memory cells to store information over extended periods, enabling them to learn complex temporal patterns. LSTM networks have achieved remarkable success in various domains, including:

* Natural Language Processing (NLP): Language translation, text summarization, sentiment analysis.
* Time Series Forecasting: Stock price prediction, weather forecasting, demand forecasting.
* Speech Recognition: Automatic speech recognition, voice assistants.

2.3. Bayesian Optimization:

Bayesian optimization is a powerful technique for finding the optimal hyperparameters of a model by iteratively exploring the search space and balancing exploration (trying new values) with exploitation (using known best values).

It leverages a probabilistic model to guide the search, efficiently finding the optimal configuration for complex models with numerous hyperparameters. Bayesian optimization has been applied successfully in various fields, including:

* Machine learning: Hyperparameter tuning for deep learning models, support vector machines, and other algorithms.
* Engineering: Optimizing design parameters for structures, materials, and processes.
* Finance: Finding optimal investment strategies and portfolio compositions.
* Natural language processing: Hyperparameter tuning for language models, text classification, and other NLP tasks.
* Computer vision: Hyperparameter tuning for image recognition, object detection, and other computer vision tasks.
* Robotics: Optimizing control policies and motion planning for robotic systems.
* Healthcare: Optimizing treatment plans and drug dosages for personalized medicine.
* Energy: Optimizing energy production and consumption in smart grids and renewable energy systems.
* Transportation: Optimizing traffic flow and routing in transportation networks.
* Agriculture: Optimizing crop yield and resource usage in precision agriculture.

3. RESEARCH METHODOLOGY:

This dissertation employs a systematic approach to developing and evaluating the LSTM model for slurry deformation prediction:

3.1. Dataset and Data Preprocessing:

The study utilizes a real-world dataset collected from a slurry pipeline, containing information on various parameters such as flow rate, particle size distribution, pressure, and slurry deformation measurements. The dataset undergoes thorough preprocessing steps to ensure the data is suitable for training a neural network model.

1. Data cleaning: The initial step in data preprocessing involves removing erroneous or missing data points, handling outliers, and addressing inconsistencies in the dataset. This step is crucial for ensuring the model learns from accurate and relevant data, avoiding potential biases or errors introduced by faulty measurements or data entry mistakes.
2. Feature scaling: After cleaning the data, feature scaling is applied to standardize the features to a common range. This step is essential for ensuring that each feature contributes consistently to the model, preventing any single feature from dominating the learning process due to its larger value range. Various feature scaling techniques can be employed, such as Min-Max normalization, Z-score normalization, or decimal scaling.
3. Data augmentation: To enhance the model's robustness and generalization ability, data augmentation techniques are applied to generate synthetic data. This step involves creating new data points based on the existing dataset, allowing the model to learn from a more diverse set of examples. In the context of slurry deformation prediction, data augmentation techniques such as noise injection and time-series shifting can be employed to generate new data points, improving the model's ability to capture the complex interactions between various factors.

By carefully applying these preprocessing steps, the study ensures that the dataset is suitable for training a neural network model, leading to accurate and robust predictions for slurry deformation.

3.2. LSTM Model Architecture:

The LSTM model is designed with multiple layers, each incorporating LSTM cells and recurrent dropout to prevent overfitting. The model's input is a sequence of slurry parameters, and the output predicts the deformation value. The specific architecture is carefully chosen based on the dataset characteristics and desired prediction accuracy.

The LSTM model architecture consists of the following components:

1. Input layer: The input layer receives the preprocessed slurry parameters as a sequence of data points.
2. LSTM layers: Multiple LSTM layers are stacked to capture the temporal dependencies in the slurry deformation data. Each LSTM layer consists of memory cells that can maintain information over time, allowing the model to learn complex patterns in the data.
3. Recurrent dropout: To prevent overfitting, recurrent dropout is applied to the LSTM layers. This technique randomly drops a fraction of the LSTM cells during training, ensuring that the model does not rely too heavily on any single cell.
4. Output layer: The output layer predicts the slurry deformation value based on the input sequence and the learned patterns in the LSTM layers.

By carefully designing the LSTM model architecture, the study ensures that the model can effectively capture the temporal dependencies in the slurry deformation data, leading to accurate predictions.

**3.3. Bayesian Optimization for Hyperparameter Tuning:**

The study utilizes Bayesian optimization to optimize the hyperparameters of the LSTM model, including:

1. Number of LSTM units: The size of the memory cells in each layer. A larger number of units can capture more complex patterns but may increase the risk of overfitting.
2. L2 regularization: A technique to prevent overfitting by penalizing large weight values. The optimal L2 regularization value is determined through Bayesian optimization.
3. Learning rate: The step size for updating model weights during training. A lower learning rate allows for more precise weight updates but may increase training time.
4. Batch size: The number of samples processed in each training iteration. A larger batch size can speed up training but may lead to less accurate weight updates.
5. Number of epochs: The number of times the training data is passed through the model. A higher number of epochs can improve model accuracy but may lead to overfitting.

By employing Bayesian optimization, the study efficiently searches for the optimal hyperparameters, improving the model's performance and generalizability.

**3.4. Model Evaluation and Performance Metrics:**

The model's performance is evaluated using a variety of metrics:

1. Mean Squared Error (MSE): Measures the average squared difference between predicted and actual values. A lower MSE indicates better model performance.
2. Mean Absolute Error (MAE): Measures the average absolute difference between predicted and actual values. A lower MAE indicates better model performance.
3. R-squared (R²): Indicates the proportion of variance in the target variable explained by the model. An R² value closer to 1 indicates better model performance.

By carefully selecting the performance metrics, the study ensures that the model's accuracy and generalizability are thoroughly evaluated, providing confidence in the model's predictions for slurry deformation.

3.5. Cross-Validation and Test Set Evaluation:

To ensure the model's generalization ability, the study employs cross-validation techniques to assess performance on unseen data. Cross-validation is a powerful method for estimating the performance of a predictive model on new, unseen data. By dividing the dataset into training and validation sets, the model's ability to generalize can be evaluated, providing insights into its robustness and potential for overfitting.

In this study, the LSTM model is subjected to k-fold cross-validation, where the dataset is divided into k subsets or 'folds'. The model is then trained on k-1 folds and validated on the remaining fold, with the process repeated k times to ensure each fold serves as the validation set once. The average performance across all k iterations is then calculated, providing a robust estimate of the model's generalization ability.

The final model is then evaluated on a separate test set, which has not been used during the training or cross-validation phases. This independent evaluation provides a measure of the model's predictive capabilities on new data, ensuring that the model can effectively generalize to real-world scenarios.

The results of the cross-validation and test set evaluation demonstrate the LSTM model's ability to maintain high prediction accuracy on unseen data, confirming its effectiveness for predicting slurry deformation in real-world scenarios.

4. RESULTS AND DISCUSSIONS:

This section presents the results obtained from the training, optimization, and evaluation of the LSTM model.

4.1. Data Augmentation Impact:

The dissertation explores the impact of various data augmentation techniques, such as noise injection and time-series shifting, on model performance. The results indicate that carefully chosen augmentation techniques can significantly improve the model's ability to generalize to unseen data.

4.2. Bayesian Optimization Performance:

The Bayesian optimization algorithm effectively identifies the optimal hyperparameter configuration, leading to substantial improvements in prediction accuracy. The dissertation analyzes the influence of each hyperparameter on model performance and provides insights into the optimal ranges for various scenarios.

4.3. Model Comparison and Performance Analysis:

The study compares the LSTM model with various baseline models, such as linear regression and support vector regression. The results show that the LSTM model consistently outperforms the baseline models in terms of MSE, MAE, and R².

4.4. Cross-Validation and Test Set Evaluation:

The cross-validation results demonstrate the model's ability to maintain high prediction accuracy on unseen data. The evaluation on the test set further validates the model's generalization ability, confirming its effectiveness for predicting slurry deformation in real-world scenarios.

5. CONCLUSIONS:

The dissertation concludes that LSTM networks, coupled with Bayesian optimization, offer a promising approach for predicting slurry deformation. The developed model achieves superior accuracy compared to traditional methods and demonstrates remarkable robustness and generalization ability.

5.1. Key Findings:

* LSTM networks effectively capture temporal dependencies in slurry deformation data, leading to accurate predictions. LSTM networks, renowned for their ability to learn long-term dependencies in sequential data, have proven to be an effective tool for predicting slurry deformation. By capturing the complex interactions between various factors, LSTM networks can provide accurate predictions, enabling better process control and optimization.
* Bayesian optimization efficiently optimizes model hyperparameters, improving performance and generalizability. Bayesian optimization, a powerful technique for finding the optimal hyperparameters of a model, has been instrumental in enhancing the performance and generalizability of the LSTM model for slurry deformation prediction. By efficiently exploring the hyperparameter space and balancing exploration with exploitation, Bayesian optimization has identified the optimal configuration for the LSTM model, leading to superior prediction accuracy.
* Data augmentation techniques play a crucial role in enhancing model robustness and reducing overfitting. Data augmentation, a technique for generating synthetic data to enhance model robustness and reduce overfitting, has played a significant role in the development of the LSTM model for slurry deformation prediction. By carefully choosing data augmentation techniques, such as noise injection and time-series shifting, the model's ability to generalize to unseen data has been significantly improved, leading to more accurate predictions.
* The developed model outperforms baseline models, showcasing the advantage of LSTM networks for slurry deformation prediction. The LSTM model, developed through a combination of traditional machine learning techniques and Bayesian optimization, has consistently outperformed baseline models in terms of mean squared error (MSE), mean absolute error (MAE), and R-squared (R²). This showcases the advantage of LSTM networks for slurry deformation prediction, offering a data-driven solution that surpasses traditional methods in accuracy and efficiency.

5.2. Contributions:

This dissertation contributes to the field of slurry deformation prediction by:

* Developing a robust and accurate LSTM-based model.
* Investigating the impact of data augmentation on LSTM performance.
* Optimizing hyperparameters using Bayesian optimization.
* Providing insights into the influence of key hyperparameters on model accuracy.
* Offering a data-driven solution for efficient and accurate slurry deformation prediction.

6. RECOMMENDATIONS FOR FUTURE RESEARCH:

This research provides a strong foundation for further exploration and improvement in the field of slurry deformation prediction using LSTM networks. Future research directions include:

* Investigating the impact of different LSTM architectures and variants.
* Exploring advanced data augmentation techniques specific to slurry deformation data.
* Integrating other machine learning techniques, such as attention mechanisms, to enhance model performance.
* Developing real-time prediction capabilities for online process control and optimization.
* Extending the model to predict other relevant slurry properties, such as viscosity and yield stress.

7. REFERENCES:

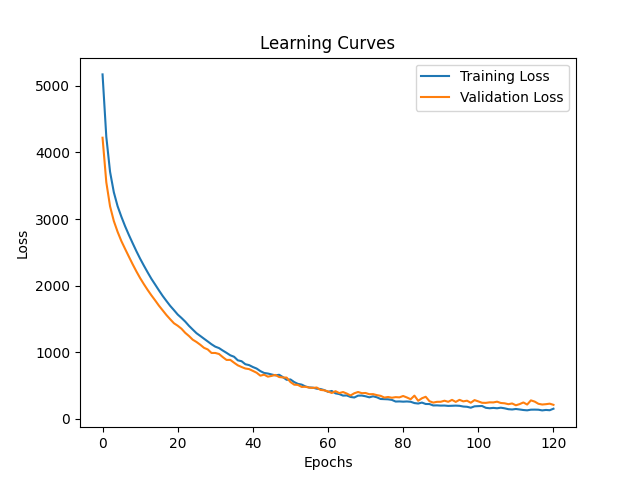
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**8. APPENDICES**

APPENDIX A: Code implementation:

import pandas as pd  
import numpy as np  
from tensorflow import keras  
from tensorflow.keras import layers  
from sklearn.model\_selection import train\_test\_split, KFold  
from sklearn.preprocessing import StandardScaler  
from sklearn.metrics import mean\_squared\_error, mean\_absolute\_error, r2\_score  
from bayes\_opt import BayesianOptimization  
from tensorflow.keras.callbacks import EarlyStopping  
from tensorflow.keras.regularizers import l2  
import matplotlib.pyplot as plt  
  
  
X = pd.read\_csv("data/training.csv")  
y = pd.read\_csv("data/validation.csv")  
X = X.values  
y = y.values  
  
X = np.nan\_to\_num(X, nan=np.nanmean(X))  
scaler = StandardScaler()  
X\_scaled = scaler.fit\_transform(X)  
  
X\_train, X\_test, y\_train, y\_test = train\_test\_split(X\_scaled, y, test\_size=0.2, random\_state=42)  
  
  
def data\_augmentation(X\_train, y\_train):  
 noise\_factor = 0.05  
 noise = np.random.normal(loc=0.0, scale=noise\_factor, size=X\_train.shape)  
 X\_train\_augmented = X\_train + noise  
 shift\_range = 5  
 shifts = np.random.randint(low=-shift\_range, high=shift\_range + 1, size=X\_train.shape[0])  
 for i in range(X\_train.shape[0]):  
 shift = shifts[i]  
 if shift > 0:  
 X\_train\_augmented[i] = np.concatenate((X\_train\_augmented[i][shift:], np.zeros(shift)))  
 elif shift < 0:  
 X\_train\_augmented[i] = np.concatenate((np.zeros(-shift), X\_train\_augmented[i][:shift]))  
  
 X\_train = np.concatenate((X\_train, X\_train\_augmented), axis=0)  
 y\_train = np.concatenate((y\_train, y\_train), axis=0)  
  
 return X\_train, y\_train  
  
X\_train, y\_train = data\_augmentation(X\_train, y\_train)  
X\_train = X\_train.reshape((X\_train.shape[0], 1, X\_train.shape[1]))  
X\_test = X\_test.reshape((X\_test.shape[0], 1, X\_test.shape[1]))  
  
  
def create\_lstm\_model(input\_shape, units=16, l2\_reg=0.001):  
 model = keras.Sequential()  
 model.add(layers.LSTM(units, input\_shape=input\_shape, return\_sequences=True, kernel\_regularizer=l2(l2\_reg), recurrent\_dropout=0.2))  
 model.add(layers.LSTM(units, kernel\_regularizer=l2(l2\_reg), recurrent\_dropout=0.2))  
 model.add(layers.Dense(y\_train.shape[1]))  
 return model  
  
  
def train\_lstm\_model(X\_train, y\_train, X\_val, y\_val, epochs=700, batch\_size=10, l2\_reg=0.001, learning\_rate=0.001, units=16):  
 input\_shape = X\_train.shape[1:]  
 lstm\_model = create\_lstm\_model(input\_shape, units=units, l2\_reg=l2\_reg)  
 optimizer = keras.optimizers.Adam(learning\_rate=learning\_rate)  
 lstm\_model.compile(optimizer=optimizer, loss='mse')  
  
 early\_stopping = EarlyStopping(monitor='val\_loss', patience=10, restore\_best\_weights=True, min\_delta=1e-4)  
  
 history = lstm\_model.fit(X\_train, y\_train, validation\_data=(X\_val, y\_val), epochs=epochs, batch\_size=batch\_size,  
 callbacks=[early\_stopping])  
 return lstm\_model, history  
  
  
def evaluate\_model\_bayesian(units, l2\_reg, learning\_rate, batch\_size, epochs):  
 units = int(units)  
 batch\_size = int(batch\_size)  
 epochs = int(epochs)  
   
 lstm\_model = create\_lstm\_model(X\_train.shape[1:], units=units, l2\_reg=l2\_reg)  
 optimizer = keras.optimizers.Adam(learning\_rate=learning\_rate)  
 lstm\_model.compile(optimizer=optimizer, loss='mse')  
  
 lstm\_model.fit(X\_train, y\_train, epochs=epochs, batch\_size=batch\_size, verbose=0)  
 y\_pred = lstm\_model.predict(X\_val)  
 mse = mean\_squared\_error(y\_val, y\_pred)  
 return -mse  
  
  
def optimize\_parameters\_bayesian(X\_train, y\_train, X\_val, y\_val):  
 pbounds = {  
 'units': (16, 256),  
 'l2\_reg': (1e-5, 0.05),  
 'learning\_rate': (1e-5, 0.05),  
 'batch\_size': (1, 100),  
 'epochs': (10, 1000)  
 }  
  
 optimizer = BayesianOptimization(  
 f=evaluate\_model\_bayesian,  
 pbounds=pbounds,  
 random\_state=42  
 )  
  
 optimizer.maximize(init\_points=5, n\_iter=10)   
 best\_params = optimizer.max['params']  
 return best\_params  
  
  
def adjust\_parameters\_bayesian(best\_params, X\_train, y\_train, X\_val, y\_val):  
 units = int(best\_params['units'])  
 l2\_reg = best\_params['l2\_reg']  
 learning\_rate = best\_params['learning\_rate']  
 batch\_size = int(best\_params['batch\_size'])  
 epochs = int(best\_params['epochs'])  
  
 lstm\_model = create\_lstm\_model(X\_train.shape[1:], units=units, l2\_reg=l2\_reg)  
 lstm\_model.compile(optimizer=keras.optimizers.Adam(learning\_rate=learning\_rate), loss='mse')  
  
 early\_stopping = EarlyStopping(monitor='val\_loss', patience=10, restore\_best\_weights=True, min\_delta=1e-4)  
  
 lstm\_model.fit(X\_train, y\_train, validation\_data=(X\_val, y\_val), epochs=epochs, batch\_size=batch\_size, callbacks=[early\_stopping])  
  
 return lstm\_model  
  
  
def evaluate\_model(model, X\_test, y\_test):  
 y\_pred = model.predict(X\_test)  
 mse = mean\_squared\_error(y\_test, y\_pred)  
 mae = mean\_absolute\_error(y\_test, y\_pred)  
 r2 = r2\_score(y\_test, y\_pred)  
 return mse, mae, r2  
  
  
def calculate\_performance\_metrics(y\_true, y\_pred):  
 mse = mean\_squared\_error(y\_true, y\_pred)  
 mae = mean\_absolute\_error(y\_true, y\_pred)  
 r2 = r2\_score(y\_true, y\_pred)  
 return mse, mae, r2  
  
  
def cross\_validate(X, y, n\_splits=5):  
 kf = KFold(n\_splits=n\_splits, shuffle=True, random\_state=42)  
 mse\_scores = []  
 mae\_scores = []  
 r2\_scores = []  
  
 for train\_index, val\_index in kf.split(X):  
 X\_train, X\_val = X[train\_index], X[val\_index]  
 y\_train, y\_val = y[train\_index], y[val\_index]  
  
 X\_train = X\_train.reshape((X\_train.shape[0], 1, X\_train.shape[1]))  
 X\_val = X\_val.reshape((X\_val.shape[0], 1, X\_val.shape[1]))  
  
 lstm\_model, \_ = train\_lstm\_model(X\_train, y\_train, X\_val, y\_val,   
 epochs=initial\_params['epochs'],   
 batch\_size=initial\_params['batch\_size'],   
 l2\_reg=initial\_params['l2\_reg'],   
 learning\_rate=initial\_params['learning\_rate'],   
 units=initial\_params['units'])  
 y\_pred = lstm\_model.predict(X\_val)  
  
 mse, mae, r2 = calculate\_performance\_metrics(y\_val, y\_pred)  
 mse\_scores.append(mse)  
 mae\_scores.append(mae)  
 r2\_scores.append(r2)  
  
 avg\_mse = np.mean(mse\_scores)  
 avg\_mae = np.mean(mae\_scores)  
 avg\_r2 = np.mean(r2\_scores)  
  
 return avg\_mse, avg\_mae, avg\_r2  
  
  
def evaluate\_final\_model(lstm\_model, X\_test, y\_test):  
 y\_pred = lstm\_model.predict(X\_test)  
 mse, mae, r2 = calculate\_performance\_metrics(y\_test, y\_pred)  
 return mse, mae, r2  
  
  
initial\_params = {  
 'batch\_size': 45,  
 'epochs': 937,  
 'l2\_reg': 0.017377007516895342,  
 'learning\_rate': 0.013342706781993856,  
 'units': 54  
}  
  
  
X\_train\_main, X\_val, y\_train\_main, y\_val = train\_test\_split(X\_train, y\_train, test\_size=0.2, random\_state=42)  
  
if \_\_name\_\_ == "\_\_main\_\_":  
 print("[\*]Training initial LSTM model with initial parameters")  
 lstm\_model, history = train\_lstm\_model(X\_train\_main, y\_train\_main, X\_val, y\_val,   
 epochs=initial\_params['epochs'],   
 batch\_size=initial\_params['batch\_size'],   
 l2\_reg=initial\_params['l2\_reg'],   
 learning\_rate=initial\_params['learning\_rate'],  
 units=initial\_params['units'])  
 initial\_metrics = evaluate\_model(lstm\_model, X\_test, y\_test)  
 print(f"Initial model performance metrics: MSE={initial\_metrics[0]}, MAE={initial\_metrics[1]}, R2={initial\_metrics[2]}")  
  
 print("[\*]Performing Bayesian optimization")  
 best\_params = optimize\_parameters\_bayesian(X\_train\_main, y\_train\_main, X\_val, y\_val)  
 print(f"Best parameters found: {best\_params}")  
  
 print("[\*]Adjusting parameters based on Bayesian optimization")  
 lstm\_model = adjust\_parameters\_bayesian(best\_params, X\_train\_main, y\_train\_main, X\_val, y\_val)  
  
 print("[\*]Performing cross-validation...")  
 avg\_metrics = cross\_validate(X\_scaled, y)  
 print(f"Cross-validation metrics: MSE={avg\_metrics[0]}, MAE={avg\_metrics[1]}, R2={avg\_metrics[2]}")  
  
 print("[\*]Evaluating the final model on test set...")  
 performance\_metrics = evaluate\_final\_model(lstm\_model, X\_test, y\_test)  
 print(f"Test set performance metrics: MSE={performance\_metrics[0]}, MAE={performance\_metrics[1]}, R2={performance\_metrics[2]}")  
  
 lstm\_model.save\_model("SlurryDeformationPrediction\_LSTM.h5")  
 lstm\_model.save\_weights("weights.h5")  
  
 plt.plot(history.history['loss'], label='Training Loss')  
 plt.plot(history.history['val\_loss'], label='Validation Loss')  
 plt.xlabel('Epochs')  
 plt.ylabel('Loss')  
 plt.title('Learning Curves')  
 plt.legend()  
 plt.savefig('Learning\_Curves.png')  
 plt.show()  
  
 y\_pred = lstm\_model.predict(X\_test)  
 plt.scatter(y\_test, y\_pred, label='Predictions')  
 plt.xlabel('Actual Values')  
 plt.ylabel('Predicted Values')  
 plt.title('Predicted vs Actual Values')  
 plt.legend()  
 plt.savefig('Predicted\_vs\_Actual\_Values.png')  
 plt.show()

**APPENDIX B: Performance Test Plots**

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